Current Research:

1. The study of antiperovskites for possible applications in photocatalytic water splitting and harvesting sunlight.

2. Machine learning + semi-empirical Hamiltonian model approach for obtaining excitation energies and absorption spectra of nano-clusters.

3. In collaboration with Alex Urban (Columbia University) group, we are working on an active learning project: Optimal data sets for construction of machine learning data sets.

4. A collaborative research with Prof. Michele Pavanello Group (Rutgers University-Newark) on efficient pseudopotentials for orbital free DFT.